10608949.trn 08/24/2004

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NEWS 1		Web Page URLs for STN Seminar Schedule - N. America
NEWS 2		"Ask CAS" for self-help around the clock
NEWS 3	May 12	EXTEND option available in structure searching
NEWS 4	May 12	Polymer links for the POLYLINK command completed in REGISTRY
NEWS 5	May 27	New UPM (Update Code Maximum) field for more efficient patent SDIs in CAplus
NEWS 6	May 27	CAplus super roles and document types searchable in REGISTRY
NEWS 7	Jun 28	Additional enzyme-catalyzed reactions added to CASREACT
NEWS 8	Jun 28	ANTE, AQUALINE, BIOENG, CIVILENG, ENVIROENG, MECHENG, and WATER from CSA now available on STN(R)
NEWS 9	Jul 12	BEILSTEIN enhanced with new display and select options, resulting in a closer connection to BABS
NEWS 10	Jul 30	BEILSTEIN on STN workshop to be held August 24 in conjunction with the 228th ACS National Meeting
NEWS 11	AUG 02	IFIPAT/IFIUDB/IFICDB reloaded with new search and display fields
NEWS 12	AUG 02	CAplus and CA patent records enhanced with European and Japan Patent Office Classifications
NEWS 13	AUG 02	STN User Update to be held August 22 in conjunction with the 228th ACS National Meeting
NEWS 14	AUG 02	The Analysis Edition of STN Express with Discover! (Version 7.01 for Windows) now available
NEWS 15	AUG 04	Pricing for the Save Answers for SciFinder Wizard within STN Express with Discover! will change September 1, 2004

NEWS EXPRESS	JULY 30 CURRENT WINDOWS VERSION IS V7.01, CURRENT MACINTOSH VERSION IS V6.0c(ENG) AND V6.0Jc(JP), AND CURRENT DISCOVER FILE IS DATED 11 AUGUST 2004
NEWS HOURS	STN Operating Hours Plus Help Desk Availability
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NEWS PHONE	Direct Dial and Telecommunication Network Access to STN
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FILE 'HOME' ENTERED AT 12:03:06 ON 24 AUG 2004

=> FIL REGISTRY

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'REGISTRY' ENTERED AT 12:03:13 ON 24 AUG 2004

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 23 AUG 2004 HIGHEST RN 731771-88-3
DICTIONARY FILE UPDATES: 23 AUG 2004 HIGHEST RN 731771-88-3

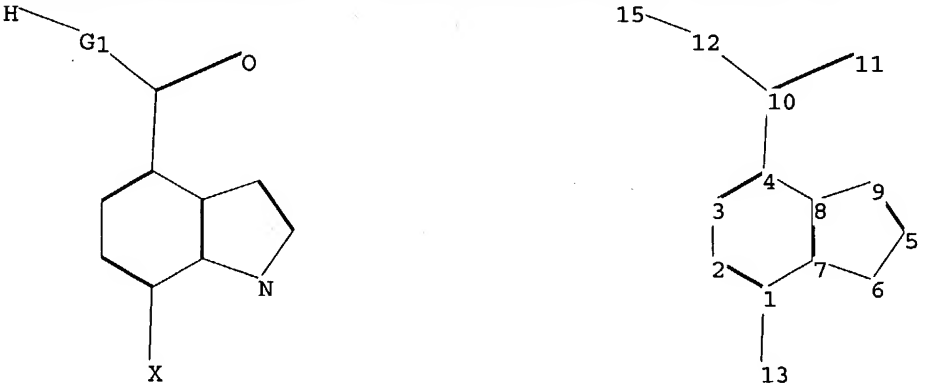
TSCA INFORMATION NOW CURRENT THROUGH MAY 21, 2004

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at:
http://www.cas.org/ONLINE/DBSS/registryss.html

=>
Uploading C:\Program Files\Stnexp\Queries\10608949.str



chain nodes :
10 11 12 13 15
ring nodes :
1 2 3 4 5 6 7 8 9
chain bonds :
1-13 4-10 10-11 10-12 12-15
ring bonds :
1-2 1-7 2-3 3-4 4-8 5-6 5-9 6-7 7-8 8-9
exact/norm bonds :
5-6 6-7 10-11 10-12 12-15
exact bonds :
1-13 4-10 5-9 8-9

normalized bonds :
1-2 1-7 2-3 3-4 4-8 7-8
isolated ring systems :
containing 1 :

G1:O,N

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS
11:CLASS 12:CLASS 13:CLASS 15:CLASS

L1 STRUCTURE UPLOADED

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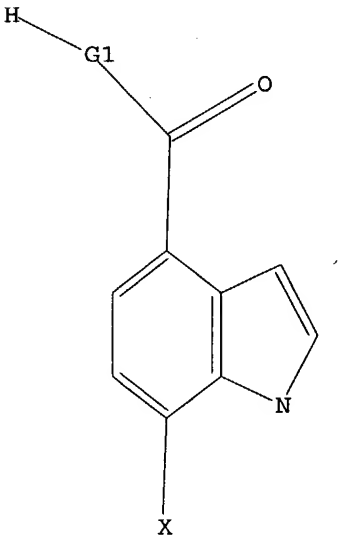
L1 HAS NO ANSWERS
L1 STR



G1 O,N

Structure attributes must be viewed using STN Express query preparation.

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SAMPLE SEARCH INITIATED 12:03:31 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 456 TO ITERATE

100.0% PROCESSED 456 ITERATIONS 3 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**
BATCH **COMPLETE**
PROJECTED ITERATIONS: 7839 TO 10401
PROJECTED ANSWERS: 3 TO 163

L2 3 SEA SSS SAM L1

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=> s l1 sss full
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FULL SCREEN SEARCH COMPLETED -   9399 TO ITERATE

100.0% PROCESSED    9399 ITERATIONS                          123 ANSWERS
SEARCH TIME: 00.00.01

L3          123 SEA SSS FUL L1

=> FIL CAPLUS
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
FULL ESTIMATED COST                               155.84     156.05

FILE 'CAPLUS' ENTERED AT 12:04:36 ON 24 AUG 2004
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FILE COVERS 1907 - 24 Aug 2004  VOL 141 ISS 9
FILE LAST UPDATED: 23 Aug 2004  (20040823/ED)

  This file contains CAS Registry Numbers for easy and accurate
  substance identification.

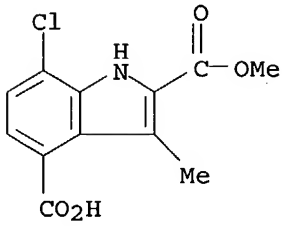
=> s l3
L4            9 L3

=> s l4 and py<=2002
      22507901 PY<=2002
L5            5 L4 AND PY<=2002

=> d l4 ibib abs hitstr tot

L4   ANSWER 1 OF 9  CAPLUS  COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER:         2004:154029  CAPLUS
DOCUMENT NUMBER:          140:423545
TITLE:                    Synthesis of the 2,3,4-trisubstituted indole fragments
                          of nosiheptide and glycothiohexide
AUTHOR(S):                Bentley, David J.; Fairhurst, John; Gallagher, Peter
                          T.; Manteuffel, Astrid K.; Moody, Christopher J.;
                          Pinder, Joanne L.
CORPORATE SOURCE:         Department of Chemistry, University of Exeter, Exeter,
                          EX4 4QD, UK
SOURCE:                   Organic & Biomolecular Chemistry (2004), 2(5), 701-708
                          CODEN: OBCRAK; ISSN: 1477-0520
PUBLISHER:                Royal Society of Chemistry
```

DOCUMENT TYPE: Journal
LANGUAGE: English
AB Two routes to the protected 4-hydroxymethyl-3-methylindole-2-carboxylate fragment of the thiopeptide antibiotic nosiheptide are described starting from Me 4-methylindole-2-carboxylate, itself prepared in two steps, or from 3-amino-4-chlorobenzoic acid. The first route can be adapted to the synthesis of a fragment of the related antibiotic glycothiohexide-α, the 3,4-bis(hydroxymethyl)indole-2-carboxylate.
IT **691362-87-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of the 2,3,4-trisubstituted indole fragments of nosiheptide and glycothiohexide)
RN 691362-87-5 CAPLUS
CN 1H-Indole-2,4-dicarboxylic acid, 7-chloro-3-methyl-, 2-methyl ester (9CI) (CA INDEX NAME)

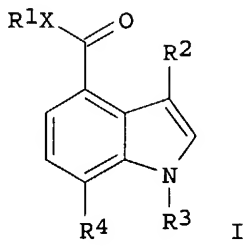


REFERENCE COUNT: 50 THERE ARE 50 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 2 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2004:142896 CAPLUS
DOCUMENT NUMBER: 140:199201
TITLE: Method of preparation of 4,7-disubstituted indoles
INVENTOR(S): Alper, Phil B.; Nguyen, Khanlinh T.
PATENT ASSIGNEE(S): Trm Llc, Bermuda
SOURCE: PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004014294	A2	20040219	WO 2003-US20395	20030627
WO 2004014294	A3	20040701		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2004110944	A1	20040610	US 2003-608949	20030626

PRIORITY APPLN. INFO.: US 2002-392804P P 20020628
US 2003-608949 A 20030626
OTHER SOURCE(S): CASREACT 140:199201; MARPAT 140:199201
GI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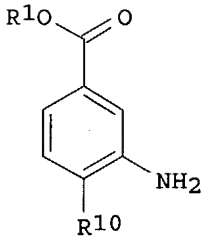
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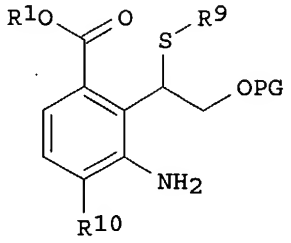
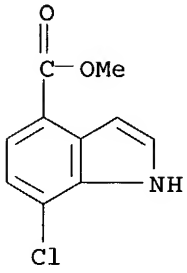

III

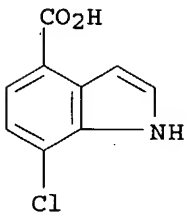
AB The invention provides a synthetic method for preparing biol. important title compds. I [wherein R1 = H or (un)substituted (cyclo)alkyl or (hetero)aryl; R2 = H, halo, COR5, or (un)substituted alkylamino; R3 = H or (un)substituted alkyl; R4 = halo, SO1-3R6, or (un)substituted (cyclo)alkyl, alkenyl, or (hetero)aryl; R5 = (un)substituted (cyclo)alkyl or (hetero)aryl; R6 = (un)substituted (cyclo)alkyl or (hetero)aryl; X = O or NR; R = H or (un)substituted alkyl; or R and R2 together with the atoms to which they are attached join to form an (un)substituted 5-, 6-, or 7-membered heterocyclic ring] by substitution of leaving groups at the 4- and 7-positions of the indole ring. The method comprises: (1) reaction of II [wherein R10 = halo or SO1-3R6; R1, R10, and X are defined above] with a sulfide R9S(CH2)2OPG [wherein R9 = (un)substituted (cyclo)alkyl or (hetero)aryl; PG = protecting group, such as pivaloyl] to give III, (2) cleavage of the protecting group and cyclization to afford the 3,4-dihydro-1H-2-benzopyran-1-one, (3) protection of the primary amine, (4) elimination of the sulfide functional group and subsequent alcoholysis to generate the pharmacophore scaffold with leaving groups at the 4- and 7-positions of the indole ring, and (5) Pd-catalyzed coupling using an aryl boronic acid to give I. For example, reaction of Me 3-amino-4-chlorobenzoate with 2-methylthioethyl pivalate (SO2Cl2, toluene, -78°; collidine; TEA, >70°; NaOMe, MeOH; trifluoroacetic anhydride, pyridine) afforded 6-chloro-3,4-dihydro-4-methylthio-5-trifluoroacetylamino-1H-2-benzopyran-1-one (32.2%). Elimination of the sulfide using H2O2 in AcOH provided the isocoumarin (73.1%), which was treated with H2SO4 in MeOH to give Me 7-chloro-1H-indole-4-carboxylate (98%). Functionalization using phenylboronic acid (Pd2dba3, P(t-Bu)3, tributylstannyl reagent, dioxane) gave 7-phenyl-1H-indole-4-carboxylic acid.

IT **503816-69-1P**, 4-Carbomethoxy-7-chloroindole
RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT

(Reactant or reagent)
(intermediate; preparation of 4,7-disubstituted indoles from aminobenzoates and sulfides)
RN 503816-69-1 CAPLUS
CN 1H-Indole-4-carboxylic acid, 7-chloro-, methyl ester (9CI) (CA INDEX NAME)



L4 ANSWER 3 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:520167 CAPLUS
DOCUMENT NUMBER: 139:214283
TITLE: Bartoli Indole Synthesis on Solid Supports
AUTHOR(S): Knepper, Kerstin; Braese, Stefan
CORPORATE SOURCE: Kekule-Institut fuer Organische Chemie and Biochemie, Rheinische Friedrich-Wilhelms-Universitaet Bonn, Bonn, D-53121, Germany
SOURCE: Organic Letters (2003), 5(16), 2829-2832
CODEN: ORLEF7; ISSN: 1523-7060
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:214283
AB Bartoli indole synthesis was performed on solid supports. Starting from Merrifield resin, immobilization of five nitrobenzoic acids was performed. Addition of four different alkenyl Grignard reagents and basic cleavage leads to substituted Me indolecarboxylates in excellent purities. Features of this reaction are the stability of halide groups, ester moieties, and tolerance of o,o'-unsubstituted nitro resins. Heck and Sonogashira reactions are also possible with immobilized indoles.
IT **588688-45-3DP**, polymer-supported **588688-46-4DP**, polymer-supported **588688-47-5DP**, polymer-supported **588688-48-6DP**, polymer-supported **588688-52-2DP**, polymer-supported **588688-53-3DP**, polymer-supported **588688-54-4DP**, polymer-supported **588688-55-5DP**, polymer-supported
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(Bartoli indole synthesis on solid supports)
RN 588688-45-3 CAPLUS
CN 1H-Indole-4-carboxylic acid, 7-chloro- (9CI) (CA INDEX NAME)



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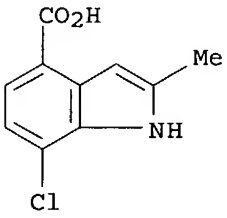

RN 588688-47-5 CAPLUS
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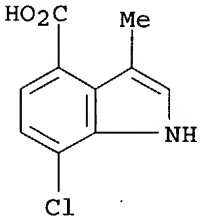

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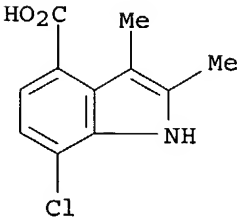

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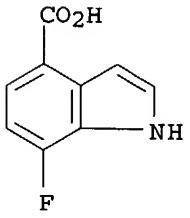

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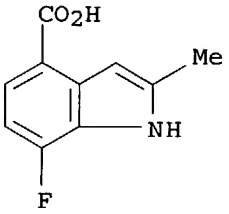

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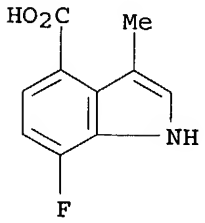

RN 588688-55-5 CAPLUS
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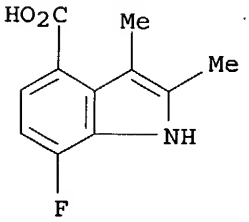

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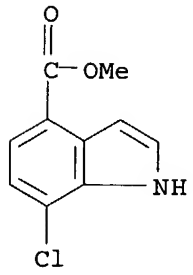
588688-36-2P 588688-40-8P 588688-41-9P
588688-42-0P 588688-43-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(Bartoli indole synthesis on solid supports)
RN 503816-69-1 CAPLUS
CN 1H-Indole-4-carboxylic acid, 7-chloro-, methyl ester (9CI) (CA INDEX

NAME)



RN 588688-34-0 CAPLUS
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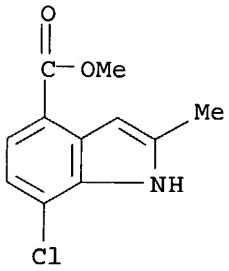

RN 588688-35-1 CAPLUS
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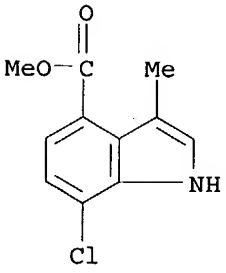

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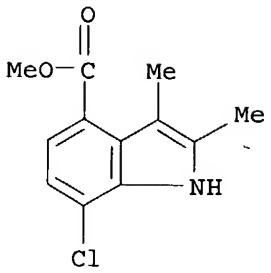

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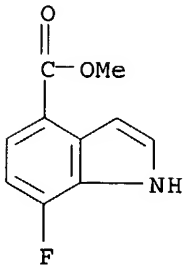

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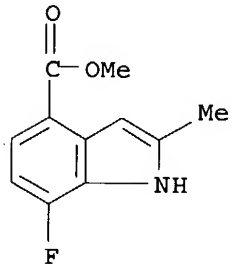

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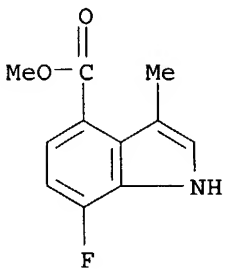
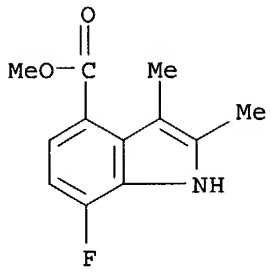
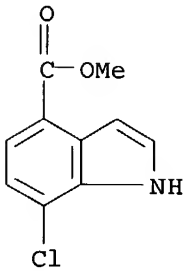


RN 588688-43-1 CAPLUS
CN 1H-Indole-4-carboxylic acid, 7-fluoro-2,3-dimethyl-, methyl ester (9CI) (CA INDEX NAME)



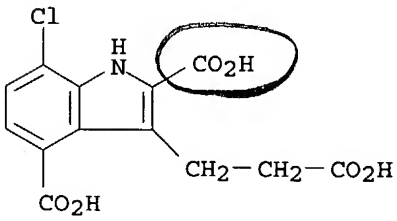
REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2003:98290 CAPLUS
DOCUMENT NUMBER: 138:287484
TITLE: Practical Synthesis and Elaboration of Methyl 7-Chloroindole-4-carboxylate
AUTHOR(S): Alper, Phil B.; Nguyen, KhanhLinh T.
CORPORATE SOURCE: The Genomics Institute, Novartis Foundation, San Diego, CA, 92121-1125, USA
SOURCE: Journal of Organic Chemistry (2003), 68(5), 2051-2053
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 138:287484
AB A synthesis of Me 7-chloroindole-4-carboxylate, a previously unknown indole derivative, is presented. The route reported herein allows for the preparation of multihundred gram quantities of material without any chromatog. purification Conditions are presented for the Pd-catalyzed elaboration of one of the diversity generating elements of this important pharmacophore.
IT **503816-69-1P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and substitution reaction of Me 7-chloroindole-4-carboxylate)
RN 503816-69-1 CAPLUS
CN 1H-Indole-4-carboxylic acid, 7-chloro-, methyl ester (9CI) (CA INDEX NAME)



REFERENCE COUNT: 63 THERE ARE 63 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:861062 CAPLUS
DOCUMENT NUMBER: 139:197300
TITLE: Product class 13: indole and its derivatives
AUTHOR(S): Joule, J. A.
CORPORATE SOURCE: Department of Chemistry, University of Manchester, Manchester, M13 9PL, UK
SOURCE: Science of Synthesis (2001), 10, 361-652
CODEN: SSCYJ9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review of preparation of indoles and its derivs. Covered reactions include cyclization, ring transformation, aromatization and substituent modifications. Subclasses covered include 1H-indol-1-ols, 1,3-dihydro-2H-indol-2-ones, and 1,2-dihydro-3H-indol-3-ones.
IT **36800-67-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(review of preparation of indoles and analogs thereof via cyclization, ring transformation, aromatization and substituent modifications)
RN 36800-67-6 CAPLUS
CN 1H-Indole-2,4-dicarboxylic acid, 3-(2-carboxyethyl)-7-chloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1348 THERE ARE 1348 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

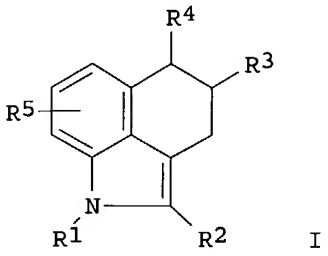
L4 ANSWER 6 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:805722 CAPLUS
DOCUMENT NUMBER: 128:34682
TITLE: Preparation of indole derivatives as cell protective agents

INVENTOR(S): Yamamoto, Ichiro; Itoh, Manabu; Shimojo, Masato; Yumiya, Yasunobu; Mukaihira, Takafumi; Akada, Yasushige
PATENT ASSIGNEE(S): Mochida Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 219 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9745410	A1	19971204	WO 1997-JP1828	19970529
W: CA, JP, KR, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
TW 430660	B	20010421	TW 1997-86107186	19970527
CA 2228268	AA	19971204	CA 1997-2228268	19970529
EP 858996	A1	19980819	EP 1997-924254	19970529
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
US 6040331	A	20000321	US 1998-11260	19980130

PRIORITY APPLN. INFO.:
JP 1996-158985 A 19960530
JP 1996-332764 A 19961128
WO 1997-JP1828 W 19970529

OTHER SOURCE(S): MARPAT 128:34682
GI



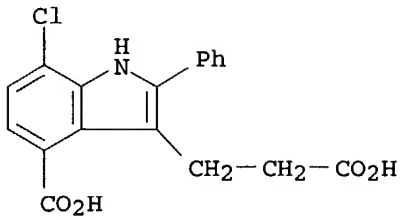
I

AB The title compds. (I; R1 = H, CO2H, alkoxycarbonyl, etc.; R2 = halo, C1-4 alkyl or alkoxy, etc.; R3, R4 = H, NR6R7; R5 = H, halo, C1-4 alkyl, etc.; R6, R7 = H, Ph, CHO, alkyl, etc.) are prepared I are useful as analgetic agents and cell protective agents for prevention and treatment of diseases accompanied by the denaturation, retraction or death of nerve cells. Thus, compound (II; X = :O) (preparation given) was treated with NH4OAc and NaBH3CN to give the title compound II (X = NH2), which at 1.0 μg/mL showed 51% inhibitory activity against death of nerve cells.

IT **199664-63-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of indole derivs. as cell protective agents)

RN 199664-63-6 CAPLUS

CN 1H-Indole-3-propanoic acid, 4-carboxy-7-chloro-2-phenyl- (9CI) (CA INDEX NAME)



L4 ANSWER 7 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1981:425087 CAPLUS
DOCUMENT NUMBER: 95:25087
TITLE: Indolobenzoxazines
INVENTOR(S): Jones, James H.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: U.S., 9 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4238486	A	19801209	US 1979-96966	19791123
EP 33767	A1	19810819	EP 1980-107206	19801120
EP 33767	B1	19840627		
R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
AT 8144	E	19840715	AT 1980-107206	19801120
DK 8004975	A	19810524	DK 1980-4975	19801121
AU 8064594	A1	19810528	AU 1980-64594	19801121
AU 539028	B2	19840906		
ES 497064	A1	19820401	ES 1980-497064	19801121
ZA 8007295	A	19820630	ZA 1980-7295	19801121
JP 56087583	A2	19810716	JP 1980-164768	19801125
JP 02027358	B4	19900615		
PRIORITY APPLN. INFO.:			US 1979-96966	19791123
			EP 1980-107206	19801120

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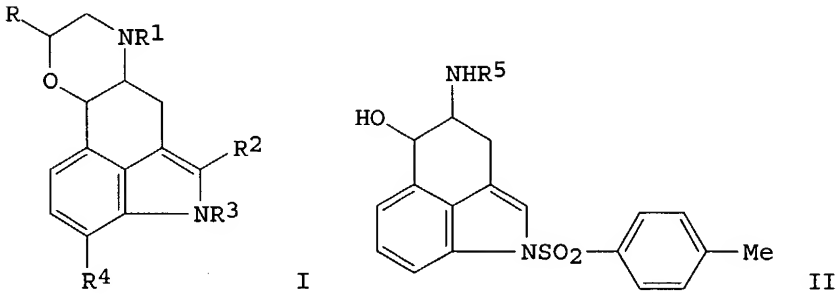


I II

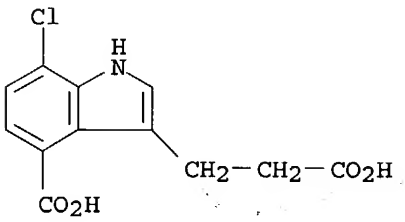
AB The indolobenzoxazines I (R = H, alkyl, aryl; R1 = H, alkyl, aralkyl, cycloalkyl, alkenyl; R2 = H, halo, alkyl; R3 = H, alkyl, aralkyl; R4 = H,

halo, alkyl, hydroxy, alkoxy) were prepared Thus, the benzindole II (R5 = H) was treated with ClCH2COCl to give II (R5 = ClCH2CO), which was cyclized followed by LiAlH4 reduction to give I (R-R4 = H). At 50-500 mg/kg I were antihypertensive, and at 20-100 mg/kg had antiparkinson and prolactin-inhibiting activity.

IT **36800-76-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of)

RN 36800-76-7 CAPLUS

CN 1H-Indole-3-propanoic acid, 4-carboxy-7-chloro- (9CI) (CA INDEX NAME)



L4 ANSWER 8 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1980:586626 CAPLUS

DOCUMENT NUMBER: 93:186626

TITLE: Preparative methods for ergoline synthons: Uhle's ketone and the C-homo analog

AUTHOR(S): Ponticello, G. S.; Baldwin, J. J.; Lumma, P. K.; McClure, D. E.

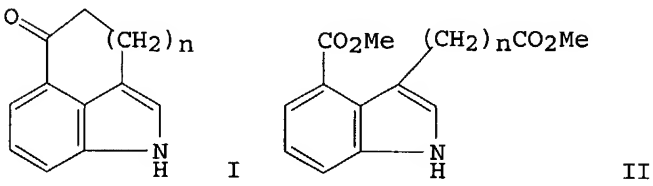
CORPORATE SOURCE: Merck Sharp and Dohme Res. Lab., Dep. Med. Chem., West Point, PA, 19486, USA

SOURCE: Journal of Organic Chemistry (1980), 45(21), 4236-8
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

GI

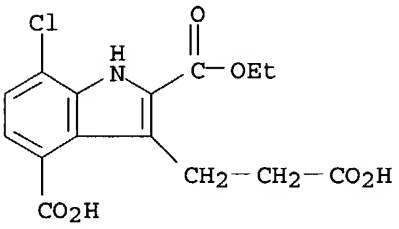


I II

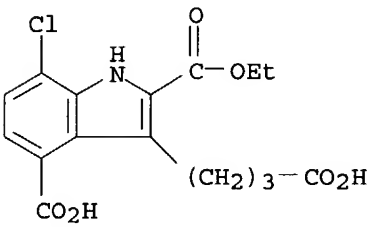
AB Preparative methods are described for the synthesis of the tricyclic indolo ketones I (n = 1, 2); these compds. are useful intermediates for the construction of ergolines and related ring systems. The synthetic strategy involves a Dieckmann cyclization-decarboxylation sequence from the diesters II (n = 2,3).

IT **36800-68-7P 74724-99-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dechlorination of)

RN 36800-68-7 CAPLUS
CN 1H-Indole-2,4-dicarboxylic acid, 3-(2-carboxyethyl)-7-chloro-, 2-ethyl ester (9CI) (CA INDEX NAME)

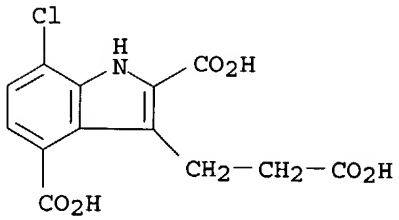


RN 74724-99-5 CAPLUS
CN 1H-Indole-2,4-dicarboxylic acid, 3-(3-carboxypropyl)-7-chloro-, 2-ethyl ester (9CI) (CA INDEX NAME)

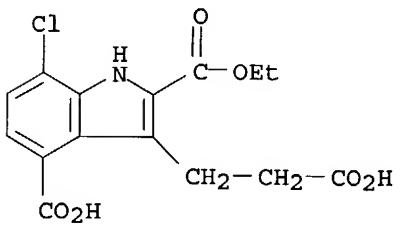


L4 ANSWER 9 OF 9 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1972:405270 CAPLUS
DOCUMENT NUMBER: 77:5270
TITLE: 1,3,4,5-Tetrahydrobenz[c,d]indoles and related compounds. I. New synthesis of 3,4-dihydrobenz[c,d]indol-5(1H)-one (Uhle's ketone)
AUTHOR(S): Bowman, R. E.; Goodburn, T. G.; Reynolds, A. A.
CORPORATE SOURCE: Res. Dev. Div., Parke Davis and Co., Pontypool, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) (1972), (9-10), 1121-3
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 77:5270
GI For diagram(s), see printed CA Issue.
AB -Carboxy-2-chlorobenzenediazonium chloride reacted with Et 2-oxocyclopentanecarboxylate followed by hydrolysis to give 1-Et H 2-oxohexanedioate (5-carboxy-2-chlorophenyl)hydrazone (I). Treatment of I with BF3.AcOH in AcOH at 90° gave 81% 4-carboxy-7-chloro-2-(ethoxycarbonyl)indole-3-propionic acid, which was converted in 67% overall yield to 4-carboxyindole-3-propionic acid (II) by sequential hydrolysis, hydrogenolysis, and thermal decarboxylation. II was readily converted to Uhle's ketone (III) by standard methods.
IT **36800-67-6P 36800-68-7P 36800-76-7P 36800-77-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 36800-67-6 CAPLUS

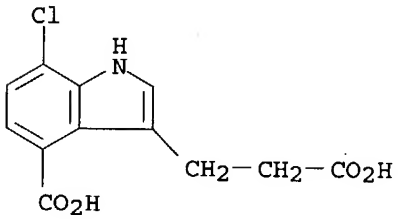
CN 1H-Indole-2,4-dicarboxylic acid, 3-(2-carboxyethyl)-7-chloro- (9CI) (CA INDEX NAME)



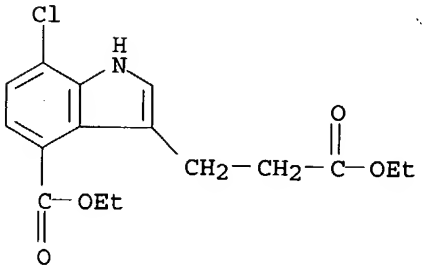
RN 36800-68-7 CAPLUS
CN 1H-Indole-2,4-dicarboxylic acid, 3-(2-carboxyethyl)-7-chloro-, 2-ethyl ester (9CI) (CA INDEX NAME)



RN 36800-76-7 CAPLUS
CN 1H-Indole-3-propanoic acid, 4-carboxy-7-chloro- (9CI) (CA INDEX NAME)



RN 36800-77-8 CAPLUS
CN 1H-Indole-3-propanoic acid, 7-chloro-4-(ethoxycarbonyl)-, ethyl ester (9CI) (CA INDEX NAME)



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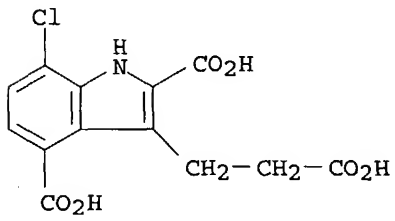
L5 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2002:861062 CAPLUS
DOCUMENT NUMBER: 139:197300
TITLE: Product class 13: indole and its derivatives
AUTHOR(S): Joule, J. A.
CORPORATE SOURCE: Department of Chemistry, University of Manchester, Manchester, M13 9PL, UK
SOURCE: Science of Synthesis (**2001**), 10, 361-652
CODEN: SSCYJ9
PUBLISHER: Georg Thieme Verlag
DOCUMENT TYPE: Journal; General Review
LANGUAGE: English
AB A review of preparation of indoles and its derivs. Covered reactions include cyclization, ring transformation, aromatization and substituent modifications. Subclasses covered include 1H-indol-1-ols, 1,3-dihydro-2H-indol-2-ones, and 1,2-dihydro-3H-indol-3-ones.
IT **36800-67-6P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(review of preparation of indoles and analogs thereof via cyclization, ring transformation, aromatization and substituent modifications)
RN 36800-67-6 CAPLUS
CN 1H-Indole-2,4-dicarboxylic acid, 3-(2-carboxyethyl)-7-chloro- (9CI) (CA INDEX NAME)



REFERENCE COUNT: 1348 THERE ARE 1348 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1997:805722 CAPLUS
DOCUMENT NUMBER: 128:34682
TITLE: Preparation of indole derivatives as cell protective agents
INVENTOR(S): Yamamoto, Ichiro; Itoh, Manabu; Shimojo, Masato; Yumiya, Yasunobu; Mukaihira, Takafumi; Akada, Yasushige
PATENT ASSIGNEE(S): Mochida Pharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 219 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

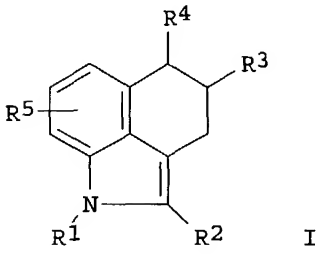
WO 9745410	A1	19971204	WO 1997-JP1828	19970529 <--
W: CA, JP, KR, US				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
TW 430660	B	20010421	TW 1997-86107186	19970527 <--
CA 2228268	AA	19971204	CA 1997-2228268	19970529 <--
EP 858996	A1	19980819	EP 1997-924254	19970529 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
US 6040331	A	20000321	US 1998-11260	19980130 <--

PRIORITY APPLN. INFO.:

JP 1996-158985	A	19960530
JP 1996-332764	A	19961128
WO 1997-JP1828	W	19970529

OTHER SOURCE(S): MARPAT 128:34682

GI



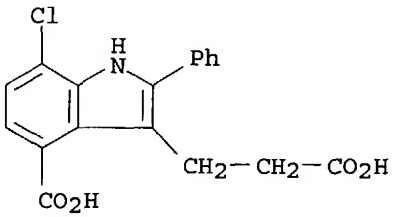
I

AB The title compds. (I; R1 = H, CO2H, alkoxycarbonyl, etc.; R2 = halo, C1-4 alkyl or alkoxy, etc.; R3, R4 = H, NR6R7; R5 = H, halo, C1-4 alkyl, etc.; R6, R7 = H, Ph, CHO, alkyl, etc.) are prepared I are useful as analgetic agents and cell protective agents for prevention and treatment of diseases accompanied by the denaturation, retraction or death of nerve cells. Thus, compound (II; X = :O) (preparation given) was treated with NH4OAc and NaBH3CN to give the title compound II (X = NH2), which at 1.0 μg/mL showed 51% inhibitory activity against death of nerve cells.

IT **199664-63-6P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of indole derivs. as cell protective agents)

RN 199664-63-6 CAPLUS

CN 1H-Indole-3-propanoic acid, 4-carboxy-7-chloro-2-phenyl- (9CI) (CA INDEX NAME)



L5 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1981:425087 CAPLUS

DOCUMENT NUMBER: 95:25087

TITLE: Indolobenzoxazines
INVENTOR(S): Jones, James H.
PATENT ASSIGNEE(S): Merck and Co., Inc., USA
SOURCE: U.S., 9 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4238486	A	19801209	US 1979-96966	19791123 <--
EP 33767	A1	19810819	EP 1980-107206	19801120 <--
EP 33767	B1	19840627		
R: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE				
AT 8144	E	19840715	AT 1980-107206	19801120 <--
DK 8004975	A	19810524	DK 1980-4975	19801121 <--
AU 8064594	A1	19810528	AU 1980-64594	19801121 <--
AU 539028	B2	19840906		
ES 497064	A1	19820401	ES 1980-497064	19801121 <--
ZA 8007295	A	19820630	ZA 1980-7295	19801121 <--
JP 56087583	A2	19810716	JP 1980-164768	19801125 <--
JP 02027358	B4	19900615		
PRIORITY APPLN. INFO.:			US 1979-96966	19791123
			EP 1980-107206	19801120

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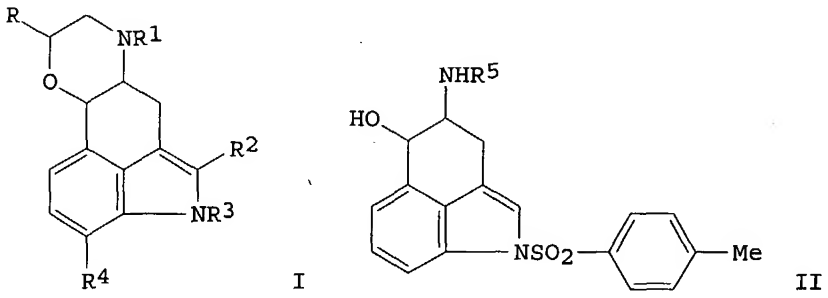


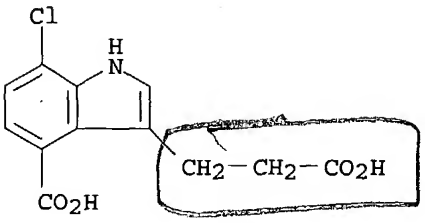
I II

AB The indolobenzoxazines I (R = H, alkyl, aryl; R1 = H, alkyl, aralkyl, cycloalkyl, alkenyl; R2 = H, halo, alkyl; R3 = H, alkyl, aralkyl; R4 = H, halo, alkyl, hydroxy, alkoxy) were prepared Thus, the benzindole II (R5 = H) was treated with ClCH2COCl to give II (R5 = ClCH2CO), which was cyclized followed by LiAlH4 reduction to give I (R-R4 = H). At 50-500 mg/kg I were antihypertensive, and at 20-100 mg/kg had antiparkinson and prolactin-inhibiting activity.

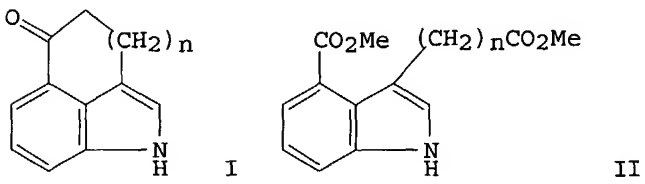
IT **36800-76-7**
RL: RCT (Reactant); RACT (Reactant or reagent)
(cyclization of)

RN 36800-76-7 CAPLUS

CN 1H-Indole-3-propanoic acid, 4-carboxy-7-chloro- (9CI) (CA INDEX NAME)



L5 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1980:586626 CAPLUS
DOCUMENT NUMBER: 93:186626
TITLE: Preparative methods for ergoline synthons: Uhle's ketone and the C-homo analog
AUTHOR(S): Ponticello, G. S.; Baldwin, J. J.; Lumma, P. K.; McClure, D. E.
CORPORATE SOURCE: Merck Sharp and Dohme Res. Lab., Dep. Med. Chem., West Point, PA, 19486, USA
SOURCE: Journal of Organic Chemistry (1980), 45(21), 4236-8
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

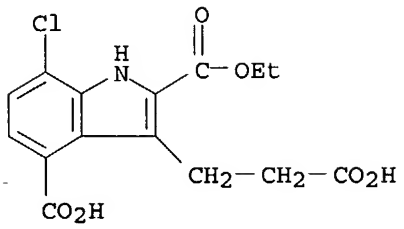


AB Preparative methods are described for the synthesis of the tricyclic indolo ketones I (n = 1, 2); these compds. are useful intermediates for the construction of ergolines and related ring systems. The synthetic strategy involves a Dieckmann cyclization-decarboxylation sequence from the diesters II (n = 2,3).

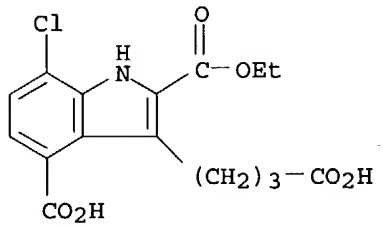
IT **36800-68-7P 74724-99-5P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and dechlorination of)

RN 36800-68-7 CAPLUS

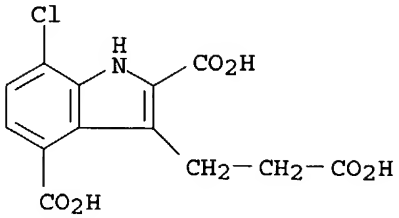
CN 1H-Indole-2,4-dicarboxylic acid, 3-(2-carboxyethyl)-7-chloro-, 2-ethyl ester (9CI) (CA INDEX NAME)



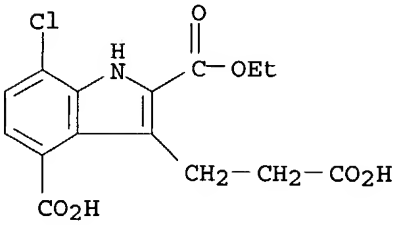
RN 74724-99-5 CAPLUS
CN 1H-Indole-2,4-dicarboxylic acid, 3-(3-carboxypropyl)-7-chloro-, 2-ethyl ester (9CI) (CA INDEX NAME)



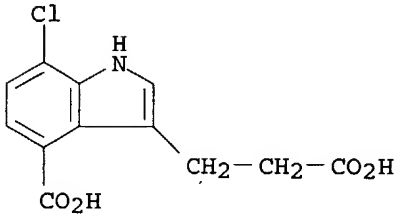
L5 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1972:405270 CAPLUS
DOCUMENT NUMBER: 77:5270
TITLE: 1,3,4,5-Tetrahydrobenz[c,d]indoles and related compounds. I. New synthesis of 3,4-dihydrobenz[c,d]indol-5(1H)-one (Uhle's ketone)
AUTHOR(S): Bowman, R. E.; Goodburn, T. G.; Reynolds, A. A.
CORPORATE SOURCE: Res. Dev. Div., Parke Davis and Co., Pontypool, UK
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1972-1999) ( ) **1972**), (9-10), 1121-3
CODEN: JCPRB4; ISSN: 0300-922X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 77:5270
GI For diagram(s), see printed CA Issue.
AB -Carboxy-2-chlorobenzenediazonium chloride reacted with Et 2-oxocyclopentanecarboxylate followed by hydrolysis to give 1-Et H 2-oxohexanedioate (5-carboxy-2-chlorophenyl)hydrazone (I). Treatment of I with BF3.AcOH in AcOH at 90° gave 81% 4-carboxy-7-chloro-2-(ethoxycarbonyl)indole-3-propionic acid, which was converted in 67% overall yield to 4-carboxyindole-3-propionic acid (II) by sequential hydrolysis, hydrogenolysis, and thermal decarboxylation. II was readily converted to Uhle's ketone (III) by standard methods.
IT **36800-67-6P 36800-68-7P 36800-76-7P 36800-77-8P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
RN 36800-67-6 CAPLUS
CN 1H-Indole-2,4-dicarboxylic acid, 3-(2-carboxyethyl)-7-chloro- (9CI) (CA INDEX NAME)



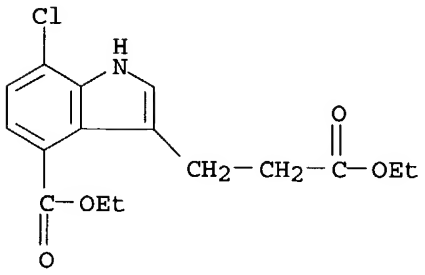
RN 36800-68-7 CAPLUS
CN 1H-Indole-2,4-dicarboxylic acid, 3-(2-carboxyethyl)-7-chloro-, 2-ethyl ester (9CI) (CA INDEX NAME)



RN 36800-76-7 CAPLUS
CN 1H-Indole-3-propanoic acid, 4-carboxy-7-chloro- (9CI) (CA INDEX NAME)



RN 36800-77-8 CAPLUS
CN 1H-Indole-3-propanoic acid, 7-chloro-4-(ethoxycarbonyl)-, ethyl ester (9CI) (CA INDEX NAME)



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COST IN U.S. DOLLARS SINCE FILE TOTAL

	ENTRY	SESSION
FULL ESTIMATED COST	69.78	225.83

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-9.80	-9.80

STN INTERNATIONAL LOGOFF AT 12:06:28 ON 24 AUG 2004